

Determination of m_c and m_b from quarkonium 1S energy levels in perturbative QCD

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Abstract

We update determination of the $\overline{\text{MS}}$ masses of the charm and bottom quarks, from comparisons of the masses of the charmonium and bottomonium 1S states with their perturbative predictions up to next-to-next-to-next-to-leading order in ϵ expansion and using the $\overline{\text{MS}}$ masses. Effects of non-zero charm-quark mass in the bottomonium masses are incorporated up to next-to-next-to-leading order. We obtain $\overline{m}_c = 1246 \pm 2(d_3) \pm 4(\alpha_s) \pm 23(\text{h.o.})$ MeV and $\overline{m}_b = 4197 \pm 2(d_3) \pm 6(\alpha_s) \pm 20(\text{h.o.}) \pm 5(m_c)$ MeV, which agree with the current Particle Data Group values.

The Standard Model (SM) of elementary particle physics has been successfully completed by the discovery of the Higgs particle, whereas no definite clue to physics beyond the SM has been found yet. In such an era, necessity for precise understanding of the SM is increasing more than ever. In particular, to meet demands for accurate measurements required in the LHC experiments as well as those for high-precision flavor physics, etc., there has been remarkable progress in the predictability of perturbative QCD in recent years. The masses of the c - and b -quarks are among the important fundamental parameters of perturbative QCD. They play crucial roles, for instance, in testing predictions of the SM for the Yukawa coupling constants of the Higgs particle, and also as the input parameters for predicting various observables in flavor physics.

The masses of the c - and b -quarks have been determined in many ways. Even referring only to works published after the latest version of Review of Particle Physics [1] by Particle Data Group (PDG) Collaboration, there are analyses based on non-relativistic QCD sum rule [2, 3], relativistic QCD sum rule [4], deep inelastic scattering [5], heavy quarkonium spectroscopy [6], and lattice computation [7]. (See [1] for earlier studies.) Their physics ingredients vary substantially, and also they probe different kinematical regions of QCD. Therefore, consistency of the determined values provides a non-trivial test of QCD, and of the SM more generally.

In this paper we determine the masses of the c - and b -quarks from comparisons of the energy levels of the charmonium and bottomonium $1S$ states with their perturbative predictions. This is an update of the mass determination performed as part of the analyses in [8, 9], which included perturbative expansion up to the next-to-next-to-leading order (NNLO). We include one more order, namely up to NNNLO. Recently, the four-loop relation to the pole and $\overline{\text{MS}}$ quark masses has been computed [10]. The present study is the first full analysis using the $\overline{\text{MS}}$ mass up to NNNLO. We also include non-zero charm-quark mass effects in the computation of the bottomonium energy levels, up to the highest order of the currently available computations (up to two loops of internal c -quark) [11]. On the experimental side, accurate data on the $\eta_c(1S)$ and $\eta_b(1S)$ masses are available today, which we include in our analysis, in addition to the $J/\psi(1S)$ and $\Upsilon(1S)$ masses used in the NNLO analyses.

The purpose of the present study is to provide another accurate determination of these quark masses, and also there is a different aspect. The heavy quarkonium states are unique among various hadrons, in that properties of individual hadronic states can be predicted purely within perturbative QCD. Hence, if we observe consistency with the masses determined by other methods with high accuracy, that can be an evidence that pure perturbative QCD is indeed capable of predicting properties of these individual hadrons with high precision, with only α_s and the quark masses as the input parameters of the theory.

Since the study at the previous order, our understanding based on perturbative QCD has developed considerably. On the one hand, developments in computational technology enabled (finally) accomplishment of the full NNNLO computation of the quarkonium energy levels, which have been carried out stepwise. Milestone computations include computations of the two-loop $1/(mr^2)$ potential [12], the full NNNLO Hamiltonian [13], the three-loop static potential [14], full formula of the spectrum [15], the four-loop relation between the pole and $\overline{\text{MS}}$ quark masses [10], etc. In addition, non-zero quark mass effects in the three-loop pole- $\overline{\text{MS}}$ mass relation have been computed [16].

On the other hand, deeper understanding on the structure of QCD has been achieved in the meantime. Solid theoretical backgrounds have been formed based on effective field theory (EFT) frameworks, such as potential-NRQCD [17] and velocity-NRQCD [18]. Accumulation of empirical facts also reinforced our understanding. There were examinations of various higher-order perturbative predictions and computations by lattice QCD simulations. New experimental data on heavy quarkonium states, such as η_c , η_b and other $c\bar{c}$, $b\bar{b}$ states, became available. Detailed comparisons of these results clarified the status of perturbative QCD predictions in an unequivocal manner [19, 14, 20, 10]. For instance, relations between renormalons and non-perturbative matrix elements in EFT became clearer, which are supported by growing number of evidences. In purely perturbative predictions, infrared (IR) contributions are encoded as IR renormalons, which induces an uncertainty of the order of non-perturbative matrix elements [21]. By contrast, in an operator product expansion (OPE) in EFT, one should subtract IR renormalons from perturbative evaluations of Wilson coefficients and replace the renormalons by non-perturbative matrix elements. (See, e.g., discussion on estimates of non-perturbative contributions to the heavy quarkonium energy levels in [22].)

Since the analysis [6] uses a method similar to ours for determination of the b -quark mass, we state the differences of our study. (1) We include the exact four-loop pole- $\overline{\text{MS}}$ mass relation [10], which became available only after the study [6]. (2) We include non-zero charm mass effects on the bottomonium energy levels up to two loops of the c -quark [11], whereas [6] includes only up to one loop. (3) Ref. [6] uses the renormalon-subtracted mass at intermediate stage, whereas we compute the energy levels directly in terms of the $\overline{\text{MS}}$ mass. (4) We use the strong coupling constant of four active quark flavors in the reference analysis of the bottomonium energy levels, in contrast to the three-flavor coupling used in [6].

Determination of c -quark mass from $J/\psi(1S)$ and $\eta_c(1S)$

In perturbative QCD, the energy level of a charmonium state is given by

$$M_{c\bar{c}} = 2m_c^{\text{pole}} + E_{\text{bin}, c\bar{c}}. \quad (1)$$

The pole mass of the c -quark is expressed in terms of the $\overline{\text{MS}}$ mass as

$$m^{\text{pole}} = \overline{m} \left[1 + \sum_{k=0}^3 d_k \left(\frac{\varepsilon \alpha_s(\overline{m})}{\pi} \right)^{k+1} + \mathcal{O}(\varepsilon^5) \right], \quad (2)$$

where $\overline{m} \equiv m^{\overline{\text{MS}}}(\overline{m}^{\overline{\text{MS}}})$ represents the $\overline{\text{MS}}$ mass renormalized at the $\overline{\text{MS}}$ mass. We use the ε -expansion [23] to cancel the $\mathcal{O}(\Lambda_{\text{QCD}})$ renormalons in $2m^{\text{pole}}$ and E_{bin} . In the computation of the charmonium levels, we use the coupling constant with $n_f = 3$ active quark flavors, $\alpha_s^{(3)}$. The values of d_k are taken from [24, 25, 10], which are converted from their values in the theory with 4 flavors (with c -quark) to those with 3 flavors (without c -quark), using the matching relation [26]

$$\alpha_s^{(n_f+1)}(\overline{m}) = \alpha_s^{(n_f)}(\overline{m}) \left[1 - \frac{11}{72} \alpha_s^{(n_f)}(\overline{m})^2 - \left(\frac{564731}{124416} - \frac{82043}{27648} \zeta(3) - \frac{2633}{31104} n_f \right) \alpha_s^{(n_f)}(\overline{m})^3 \right]. \quad (3)$$

We obtain

$$d_0 = 4/3, \quad d_1 = 10.3193, \quad d_2 = 116.300, \quad d_3 = 1687.1 \pm 21.5. \quad (4)$$

Then we express $\alpha_s(\overline{m})$ by the series expansion in $\alpha_s(\mu)$ using the relation

$$\begin{aligned} \alpha_s(\overline{m}) = \alpha_s(\mu) & \left[1 + \frac{\beta_0}{2} \log\left(\frac{\mu}{\overline{m}}\right) \left(\frac{\varepsilon\alpha_s(\mu)}{\pi}\right) \right. \\ & \left. + \left(\frac{\beta_0^2}{4} \log^2\left(\frac{\mu}{\overline{m}}\right) + \frac{\beta_1}{2} \log\left(\frac{\mu}{\overline{m}}\right) \right) \left(\frac{\varepsilon\alpha_s(\mu)}{\pi}\right)^2 + \dots \right], \end{aligned} \quad (5)$$

which follows from the renormalization-group (RG) equation for α_s ; β_i denotes the $(i+1)$ -loop coefficient of the beta function. [We suppressed the $\mathcal{O}(\varepsilon^3)$ term for brevity.] Here and hereafter, α_s represents $\alpha_s^{(n_f)}$.

The binding energy is given by [27, 28, 15]

$$E_{\text{bin}} = -\frac{4}{9}\alpha_s(\mu)^2 m^{\text{pole}} \sum_{k=0}^3 \varepsilon^{k+1} \left(\frac{\alpha_s(\mu)}{\pi}\right)^k P_k(L_\mu) + \mathcal{O}(\varepsilon^5). \quad (6)$$

Here, $P_k(L_\mu)$ is a k -th order polynomial of $L_\mu = \log[3\mu/(4\alpha_s(\mu)m^{\text{pole}})] + 1$. Apart from $c_k \equiv P_k(0)$, the polynomial is determined by the RG equation for α_s . c_k 's are given, for $J/\psi(1S)$ [$n_f = 3, n = 1, l = 0, s = 1, j = 1$], by

$$c_1 = 7/2, \quad c_2 = 142.018, \quad c_3 = 1276.83(1) + 474.289 \log \alpha_s(\mu), \quad (7)$$

and for $\eta_c(1S)$ [$n_f = 3, n = 1, l = 0, s = 0, j = 0$], by

$$c_1 = 7/2, \quad c_2 = 165.413, \quad c_3 = 908.82(1) + 597.111 \log \alpha_s(\mu). \quad (8)$$

The input value for α_s is set as [1]

$$\alpha_s^{(n_f=5)}(m_Z) = 0.1185 \pm 0.0006. \quad (9)$$

Evolving by the RG equation, it is matched to the couplings with 4 and 3 flavors successively, using the matching relation eq. (3). We compare the predictions of the $J/\psi(1S)$ and $\eta_c(1S)$ masses with the experimental data [1]:

$$M_{J/\psi(1S)}^{\text{exp}} = 3096.916 \pm 0.011 \text{ MeV}, \quad M_{\eta_c(1S)}^{\text{exp}} = 2983.6 \pm 0.7 \text{ MeV}. \quad (10)$$

The scale dependences of the predictions are shown in Fig. 1 for $J/\psi(1S)$. Those for $\eta_c(1S)$ are similar. The scale dependences decrease as the order is raised. Fig. 1 is also consistent with the expectation of renormalon dominance that the minimal sensitivity scale increases with the order [21]. We can adjust the value of \overline{m}_c to reproduce the experimental data at the minimal sensitivity scales. The central values read $\overline{m}_c = 1266 \text{ MeV}$ and 1226 MeV , respectively, for $J/\psi(1S)$ and $\eta_c(1S)$, and the minimal sensitivity scales for the predictions up to NNNLO read $\mu = 2.14 \text{ GeV}$ and 2.42 GeV , respectively. (The

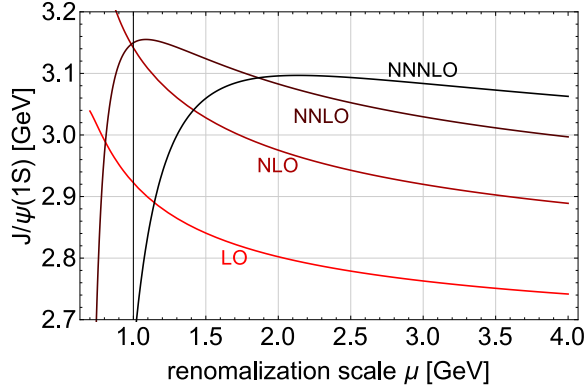


Figure 1: Scale dependences of the predictions for the $J/\psi(1S)$ mass. $N^k\text{LO}$ line represents the prediction up to $\mathcal{O}(\varepsilon^{k+1})$. We take $\overline{m}_c = 1266$ MeV, which is adjusted to reproduce the experimental data at the minimal sensitivity scale for the NNNLO line.

values of $\alpha_s(\mu)$ are 0.2712 and 0.2878, respectively.) The ε -expansions at the minimal sensitivity scales are given by

$$M_{J/\psi(1S)}^{\text{pert}} = 2532 + 263 + 170 + 109 + 23 \text{ MeV}, \quad (11)$$

$$M_{\eta_c(1S)}^{\text{pert}} = 2452 + 242 + 162 + 103 + 24 \text{ MeV}, \quad (12)$$

where the terms on the right-hand side correspond to the order $\varepsilon^0, \varepsilon^1, \dots, \varepsilon^4$ terms, respectively. They exhibit reasonably convergent behaviors.

We estimate uncertainties of our predictions, which are translated to uncertainties in the determination of \overline{m}_c . (The errors of the experimental data are negligibly small.)

(i) *Uncertainty of d_3* : The uncertainty of d_3 in eq. (4) correspond to ± 2 MeV variation of \overline{m}_c . Other uncertainties in the parameters in the expansion coefficients, such as that of c_3 , are negligibly small.

(ii) *Uncertainty of $\alpha_s(M_Z)$* : The uncertainty in the input $\alpha_s(M_Z)$ in eq. (9) corresponds to ± 4 MeV shift of \overline{m}_c .

(iii) *Uncertainty by higher-order corrections*: We estimate the uncertainty of unknown higher-order corrections in three different ways. (a) We change the scale μ from the minimal sensitivity scale to twice of that value. The corresponding variations of \overline{m}_c are about 18 MeV and 15 MeV, respectively, for $J/\psi(1S)$ and $\eta_c(1S)$. (b) We take the differences of the determined \overline{m}_c using the same method up to NNLO and NNNLO, fixing μ at the respective minimal sensitivity scales. This results in the differences of 27 MeV and 19 MeV, respectively, when we adjust $M_{c\bar{c}}$ to the $J/\psi(1S)$ and $\eta_c(1S)$ masses. (The respective minimal sensitivity scales up to NNLO are 1.08 GeV and 1.23 GeV.) (c) We take one half of the last known terms of the series in eqs. (11) and (12). This results in about 12 MeV for both states. Let us take the maximal values of (a)–(c) as our estimates of higher-order corrections. They give 27 MeV and 19 MeV for uncertainties of \overline{m}_c as determined from the masses of $J/\psi(1S)$ and $\eta_c(1S)$, respectively. The corresponding uncertainties for the predictions of $M_{c\bar{c}}(1S)$ (twice of these values) are similar in size to the estimate of uncanceled renormalon of order $\Lambda_{\text{QCD}}^3 r^2$, in the case $\Lambda_{\text{QCD}} \sim 300$ MeV

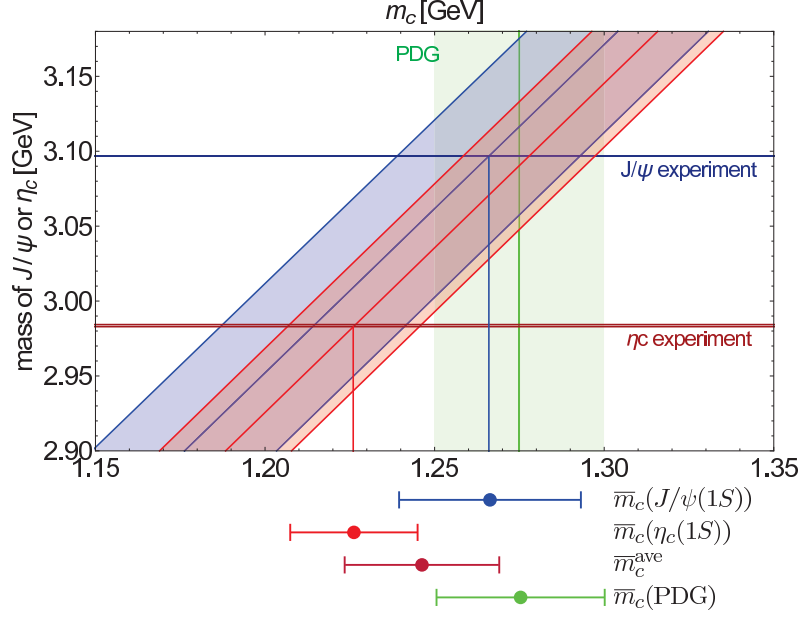


Figure 2: Determination of \overline{m}_c . Horizontal (vertical) axis represents \overline{m}_c (mass of charmonium $1S$ state). Horizontal bands denote the experimental data with errors. Diagonal bands show the perturbative QCD predictions with errors as functions of \overline{m}_c . Determined \overline{m}_c with error bars are shown below the plot. For comparison, the PDG value is also shown.

and $r \sim 1.5 \text{ GeV}^{-1}$ (although it is sensitive to the values chosen for Λ_{QCD} and r). As stated, in a purely perturbative prediction, this renormalon uncertainty is the substitute for a non-perturbative matrix element in OPE or EFT.

To summarize our results, we obtain

$$\overline{m}_c(J/\psi(1S)) = 1266 \pm 2 (d_3) \pm 4 (\alpha_s) \pm 27 (\text{h.o.}) \text{ MeV}, \quad (13)$$

$$\overline{m}_c(\eta_c(1S)) = 1226 \pm 2 (d_3) \pm 4 (\alpha_s) \pm 19 (\text{h.o.}) \text{ MeV}. \quad (14)$$

Both values are mutually consistent within the estimated errors. By taking the average of the above two estimates, we obtain

$$\overline{m}_c^{\text{ave}} = 1246 \pm 2 (d_3) \pm 4 (\alpha_s) \pm 23 (\text{h.o.}) \text{ MeV}. \quad (15)$$

It is consistent with the current PDG value $\overline{m}_c = 1275 \pm 25 \text{ MeV}$ [1]. See Fig. 2.

Determination of b -quark mass from $\Upsilon(1S)$ and $\eta_b(1S)$

In the limit where we neglect masses of quarks in internal loops, the formula for the bottomonium energy level is the same as that for the charmonium, except that we set $n_f = 4$. It is known, however, that effects of the c -quark mass is important in the predictions of the bottomonium energy levels. Presently the corrections by non-zero m_c effects are known up to $\mathcal{O}(\varepsilon^3)$. These effects are included in our predictions in the following way.

$$M_{b\bar{b}} = 2m_b^{\text{pole}} + E_{\text{bin}, b\bar{b}} \quad (16)$$

with

$$m_b^{\text{pole}} = \left[m_b^{\text{pole}} \right]_{\overline{m}_c \rightarrow 0} + \overline{m}_b \left[d_1^{(c)} \left(\frac{\varepsilon \alpha_s(\overline{m})}{\pi} \right)^2 + d_2^{(c)} \left(\frac{\varepsilon \alpha_s(\overline{m})}{\pi} \right)^3 \right], \quad (17)$$

$$E_{\text{bin}, b\bar{b}} = \left[E_{\text{bin}, b\bar{b}} \right]_{\overline{m}_c \rightarrow 0} + 2m_b^{\text{pole}} \left[-\varepsilon^2 \Delta_{\text{NLO}}^{(c)} - \varepsilon^3 \Delta_{\text{NNLO}}^{(c)} \right]. \quad (18)$$

Here, $[m_b^{\text{pole}}]_{\overline{m}_c \rightarrow 0}$ and $[E_{\text{bin}, b\bar{b}}]_{\overline{m}_c \rightarrow 0}$, respectively, represent eqs. (2) and (6) for $n_f = 4$, and the parameters therein are given by

$$d_0 = 4/3, \quad d_1 = 9.27792, \quad d_2 = 94.2137, \quad d_3 = 1220.3 \pm 21.5; \quad (19)$$

for $\Upsilon(1S)$ [$n_f = 4, n = 1, l = 0, s = 1, j = 1$],

$$c_1 = 53/18, \quad c_2 = 125.69, \quad c_3 = 1010.65(1) + 474.289 \log \alpha_s(\mu), \quad (20)$$

and for $\eta_b(1S)$ [$n_f = 4, n = 1, l = 0, s = 0, j = 0$],

$$c_1 = 53/18, \quad c_2 = 149.09, \quad c_3 = 665.70(1) + 597.111 \log \alpha_s(\mu). \quad (21)$$

The deviation from the limit $\overline{m}_c \rightarrow 0$ is parametrized as follows. At $\mathcal{O}(\varepsilon^2)$ [29, 30],

$$\begin{aligned} d_1^{(c)}(x) = & \frac{1}{18} \left[6(x+1)^2 (x^2 - x + 1) (\text{Li}_2(-x) + \log(x) \log(x+1)) \right. \\ & + 6(x-1)^2 (x^2 + x + 1) (\text{Li}_2(x) + \log(1-x) \log(x)) \\ & \left. - 6x^4 \log^2(x) - 6x^2 \log(x) - 9x^2 - \pi^2 (x^4 - 3x^3 - 3x) \right], \end{aligned} \quad (22)$$

$$\Delta_{\text{NLO}}^{(c)} = \frac{4\alpha_s(\mu)^3}{27\pi} \left[\frac{3\pi}{4} \rho - 2\rho^2 + \pi\rho^3 + \log \frac{\rho}{2} + \frac{2 - \rho^2 - 4\rho^4}{\sqrt{\rho^2 - 1}} \text{Arctan} \left(\sqrt{\frac{\rho - 1}{\rho + 1}} \right) \right], \quad (23)$$

where $x = \overline{m}_c/\overline{m}_b$ and $\rho = 3m_c^{\text{pole}}/[2\alpha_s(\mu)m_b^{\text{pole}}]$. The expressions for $d_2^{(c)}$ and $\Delta_{\text{NNLO}}^{(c)}$ are lengthy, which can be found in the original references [16] and [11], respectively, and we refrain from showing them.* We list numerical values of the parameters for some representative values of x, ρ in Tab. 1. There are no explicit spin-dependences in $d_{1,2}^{(c)}$ and $\Delta_{\text{NLO,NNLO}}^{(c)}$. Their differences between $\Upsilon(1S)$ and $\eta_b(1S)$ originate only from the different values of μ chosen to evaluate the energy levels.

After expressing $m_{b,c}^{\text{pole}}$ by $\overline{m}_{b,c}$ and applying ε -expansion, we obtain

$$\begin{aligned} M_{b\bar{b}} = & \left[M_{b\bar{b}} \right]_{\overline{m}_c \rightarrow 0} + \varepsilon^2 2\overline{m}_b \left\{ d_1^{(c)} \frac{\alpha_s^2}{\pi^2} - \Delta_{\text{NLO}}^{(c)} \right\} \\ & + \varepsilon^3 2\overline{m}_b \left\{ \left(d_2^{(c)} + 2d_1^{(c)} \cdot \frac{\beta_0}{2} \log \frac{\mu}{\overline{m}_b} \right) \frac{\alpha_s^3}{\pi^3} - \frac{2\alpha_s^4}{9\pi^2} d_1^{(c)} - \Delta_{\text{NNLO}}^{(c)} - d_0 \frac{\alpha_s}{\pi} \Delta_{\text{NLO}}^{(c)} \right\}, \end{aligned} \quad (24)$$

* Concerning $\Delta_{\text{NNLO}}^{(c)}$, while we spot misprints in eqs. (184),(186),(187) of [11], we confirm correctness of eq. (64) [apart from a ‘+’ symbol missing in the last line], which is the sum of eqs. (183)–(187).

State	μ [GeV]	$\alpha_s(\mu)$	x	ρ	$d_1^{(c)}$	$d_2^{(c)}$	$\Delta_{\text{NLO}}^{(c)}$	$\Delta_{\text{NNLO}}^{(c)}$
$\Upsilon(1S)$	5.352	0.2092	0.3050	2.187	0.4333	11.66	0.0008526	0.002348
$\eta_b(1S)$	6.157	0.2005	0.3050	2.282	0.4333	11.66	0.0007655	0.002113

Table 1: Numerical values of the parameters of non-zero charm mass effects, for representative values of the input parameters. We set $\overline{m}_b = 4.18$ GeV and $\overline{m}_c = 1.275$ GeV. We evaluate $\rho = 3x/[2\alpha_s(\mu)]$ with the $\overline{\text{MS}}$ masses; see explanation below eq. (24).

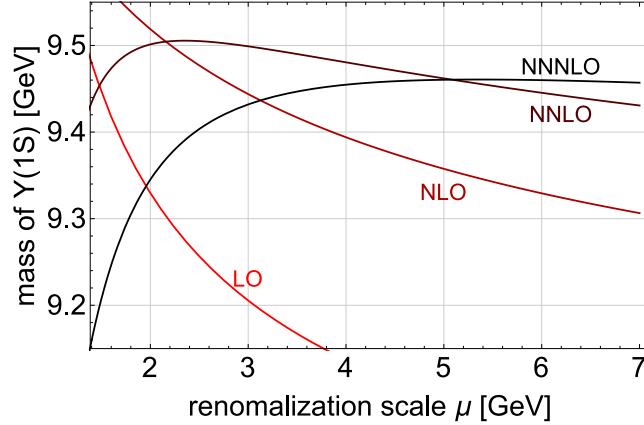


Figure 3: Scale dependences of the predictions for the $\Upsilon(1S)$ mass. We take $\overline{m}_b = 4207$ MeV. Other conventions are the same as in Fig. 1.

where we show explicitly the ε -expansion of the deviation from the $\overline{m}_c \rightarrow 0$ limit. The term proportional to $\beta_0 \log(\mu/\overline{m}_b)$ arises from rewriting $\alpha_s(\overline{m}_b)$ by $\alpha_s(\mu)$; the term proportional to $\alpha_s^4 d_1^{(c)}$ from the cross term of the leading-order binding energy and $d_1^{(c)}$; $m_{b,c}^{\text{pole}}$ in ρ are replaced by $\overline{m}_{b,c}$ without generating other terms up to the order of our interest, since the $\mathcal{O}(\varepsilon)$ terms cancel in the ratio $m_c^{\text{pole}}/m_b^{\text{pole}}$.

We compare the predictions of $\Upsilon(1S)$ and $\eta_b(1S)$ masses with the experimental data [1]:

$$M_{\Upsilon(1S)}^{\text{exp}} = 9460.30 \pm 0.26 \text{ MeV}, \quad M_{\eta_b(1S)}^{\text{exp}} = 9398.0 \pm 3.2 \text{ MeV}. \quad (25)$$

The input α_s is taken as in eq. (9). The c -quark mass in internal loops is taken as the PDG central value $\overline{m}_c = 1.275$ GeV in this analysis.[†] We adjust the value of \overline{m}_b to reproduce the experimental data. The central values read, respectively, as $\overline{m}_b = 4.207$ GeV and 4.187 GeV. The scale dependences of the predictions are shown in Fig. 3 for $\Upsilon(1S)$. Those for $\eta_b(1S)$ are similar. The minimal sensitivity scales are given by $\mu = 5.352$ GeV and 6.157 GeV, respectively. The ε -expansions at the minimal sensitivity scales are

[†] Whether we vary \overline{m}_c within the error ± 25 MeV or choose the values in eqs. (13)–(15), variations of our predictions for $M_{b\bar{b}}$ are much smaller and negligible compared to the uncertainties discussed below.

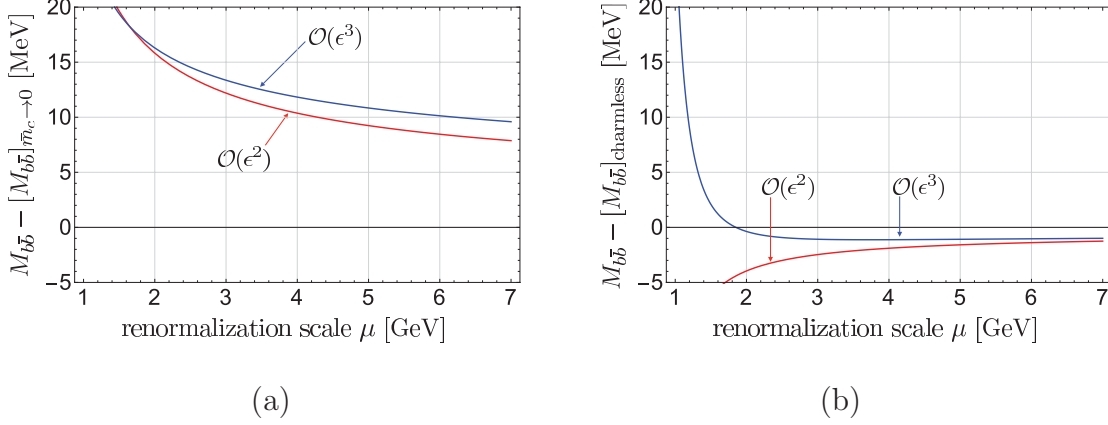


Figure 4: (a) Scale dependences of the non-zero charm mass effects for the bottomonium 1S states at $\mathcal{O}(\epsilon^2)$ and $\mathcal{O}(\epsilon^3)$. (b) Same as (a), but in the case that the energy level is reexpressed in the 3-flavor coupling $\alpha_s^{(3)}$.

given by

$$M_{\Upsilon(1S)}^{\text{pert}} = 8414 + 665 + 267 + 109 + 5 \text{ MeV}, \quad (26)$$

$$M_{\eta_b(1S)}^{\text{pert}} = 8374 + 638 + 270 + 110 + 6 \text{ MeV}. \quad (27)$$

We see reasonable stability and convergence of the predictions.

We examine separately the non-zero charm mass effects. At each order of ϵ in eq. (24), there is a cancellation inside the curly bracket, reflecting the cancellation of renormalons between $2m^{\text{pole}}$ and E_{bin} . The level of cancellation can be quantified, e.g., by the ratio of the sum of the two terms at $\mathcal{O}(\epsilon^2)$ and the sum of the absolute values of the two terms, which is about 0.3–0.4 for $2 \text{ GeV} < \mu < 6 \text{ GeV}$. The corresponding ratio at $\mathcal{O}(\epsilon^3)$ is about 0.1–0.2 for $2 \text{ GeV} < \mu < 6 \text{ GeV}$, so that the cancellation is severer.

Fig. 4(a) shows the scale dependences of the coefficients of ϵ^2 and ϵ^3 in eq. (24). They are comparable in size for $2 \text{ GeV} \lesssim \mu \lesssim 6 \text{ GeV}$. Moreover, the scale dependence increases by including the $\mathcal{O}(\epsilon^3)$ term in addition to the $\mathcal{O}(\epsilon^2)$ term. Hence, even though there are certain cancellations, we do not observe convergence and stability of the charm-mass correction by itself for the first two terms.[‡] In refs. [11, 9], an enhancement of the non-zero charm mass correction was anticipated due to an accidental scale relation $a_{1S}^{-1} \sim m_c \ll m_b$ (a_{1S} is the size of the bottomonium 1S states) and the resulting incomplete cancellation of the $\mathcal{O}(\Lambda_{\text{QCD}})$ renormalons. The above feature is consistent with this expectation, which was put forward when the full $\mathcal{O}(\epsilon^3)$ term was still unknown. In refs. [9, 6], an improvement in (apparent) convergence and stability is suggested by using the 3-flavor coupling $\alpha_s^{(3)}$ instead of $\alpha_s^{(4)}$, since the renormalon-enhanced effects are absorbed into the effective coupling $\alpha_s^{(3)}$. Indeed we confirm the improvement by this prescription. See Fig. 4(b), which shows the corresponding $\mathcal{O}(\epsilon^2)$ and $\mathcal{O}(\epsilon^3)$ terms in the $\alpha_s^{(3)}$ scheme. (We refer to [6] for the calculation method.) Here, we use the 4-flavor coupling in our reference analysis, while we use the 3-flavor coupling for an error estimate given below. This is because the c -quark cannot be regarded as completely decoupled at the scale of

[‡] Our result is also consistent with the non-zero charm mass effects found in the analyses using the non-relativistic sum rule [3], which chooses a scale $\mu \simeq 4.5 \text{ GeV}$.

the bottomonium $1S$ states [9], and to use the effective 3-flavor coupling may not be natural.

By incorporating the charm-mass effects, qualitatively the potential energy $V(r)$ between b and \bar{b} becomes steeper (interquark force becomes stronger) at large r ($\gtrsim m_c^{-1}$), due to the decoupling of the c -quark in the running of α_s [31]. This pushes up the energy levels of the bottomonium for the same input \overline{m}_b . As a result, the determined \overline{m}_b 's are reduced compared to the $m_c \rightarrow 0$ case [22] by about 8 MeV.

We estimate uncertainties in the determination of \overline{m}_b in the same way as in the charmonium case. (The errors of the experimental data are negligibly small.)

- (i) Uncertainty due to uncertainty of d_3 is ± 2 MeV.
- (ii) Uncertainty due to uncertainty of $\alpha_s(M_Z)$ is ± 6 MeV.
- (iii) Uncertainty by higher-order corrections. (a) By changing μ to twice of the value of the minimal sensitivity scale, \overline{m}_b determined from either $\Upsilon(1S)$ or $\eta_b(1S)$ varies by about 10 MeV. (b) The differences in the determined \overline{m}_b on the minimal sensitivity scales up to NNLO and NNNLO give 21 MeV and 18 MeV, respectively, for $\Upsilon(1S)$ and $\eta_b(1S)$. (c) One half of the last known terms of eqs. (26) and (27) are both about 3 MeV. We take as our estimates the maximal values of (a)–(c), namely, 21 MeV and 18 MeV, respectively, for $\Upsilon(1S)$ and $\eta_b(1S)$. Twice of these values are roughly of the same order of magnitude as (or slightly larger than) $\Lambda_{\text{QCD}}^3 r^2$, in the case $\Lambda_{\text{QCD}} \sim 300$ MeV and $r \sim 1$ GeV $^{-1}$.

In addition, we estimate uncertainties of the non-zero charm mass corrections.

- (iv) *Uncertainty of non-zero \overline{m}_c effects:* (a) The charm mass corrections at $\mathcal{O}(\varepsilon^2)$ and $\mathcal{O}(\varepsilon^3)$ shown in Fig. 4(a) are around 10 MeV at the minimal sensitivity scales $\mu \sim 5$ –6 GeV of $M_{b\bar{b}}$. We take the average of these two terms, which translates to about 5 MeV for the determined \overline{m}_b . (b) We take the difference of the determined \overline{m}_b by using the 4-flavor coupling and the 3-flavor coupling. This gives about 3 MeV for either $\Upsilon(1S)$ or $\eta_b(1S)$. We take the maximal value of (a) and (b), namely 5 MeV, as our estimate. This estimate of uncertainty from non-zero \overline{m}_c is consistent with those of previous studies [2, 3] using the non-relativistic sum rule.

To summarize our results, we obtain

$$\overline{m}_b(\Upsilon(1S)) = 4207 \pm 2 (d_3) \pm 6 (\alpha_s) \pm 21 (\text{h.o.}) \pm 5 (m_c) \text{ MeV}, \quad (28)$$

$$\overline{m}_b(\eta_b(1S)) = 4187 \pm 2 (d_3) \pm 6 (\alpha_s) \pm 18 (\text{h.o.}) \pm 5 (m_c) \text{ MeV}. \quad (29)$$

Both values are mutually consistent within the estimated errors. By taking the average of the above two estimates, we obtain

$$\overline{m}_b^{\text{ave}} = 4197 \pm 2 (d_3) \pm 6 (\alpha_s) \pm 20 (\text{h.o.}) \pm 5 (m_c) \text{ MeV}. \quad (30)$$

It is consistent with the current PDG value $\overline{m}_b = 4.18 \pm 0.03$ GeV. (See Fig. 5.)

Conclusions and discussion

We determined the c - and b -quark $\overline{\text{MS}}$ masses, by direct comparisons of the experimental data for the masses of the individual heavy quarkonium $1S$ states with the predictions of perturbative QCD. The predictions combine the state-of-the-art computational results, which are at the NNNLO level, and show stability and convergence expected for legitimate perturbative predictions. The obtained values of each mass from the different spin

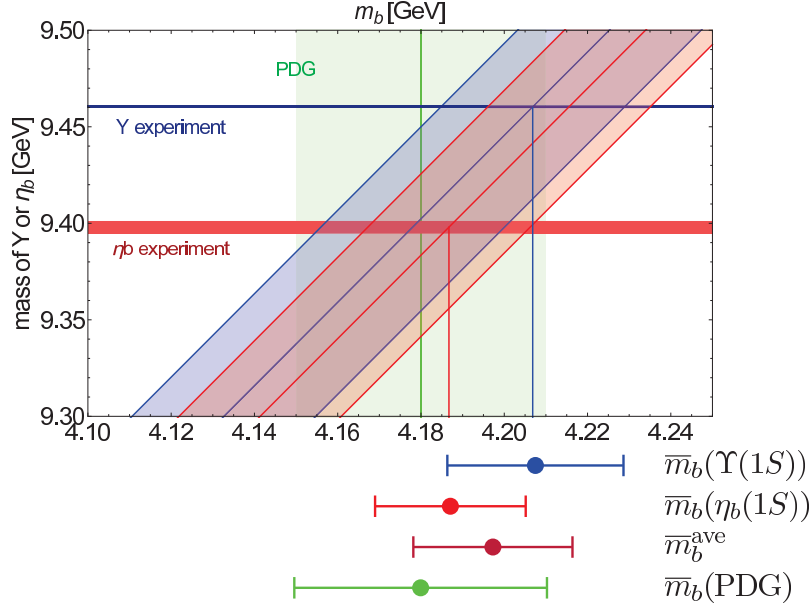


Figure 5: Determination of \overline{m}_b . Horizontal (vertical) axis represents \overline{m}_b (mass of bottomonium $1S$ state). Other notations are the same as in Fig. 2.

states are consistent with each other as well as with the current PDG value, which is determined from a wide variety of observables. The procedures of the computation and error estimates are based on fairly general prescriptions of perturbative QCD.[§]

There is a general tendency that hyperfine splittings (also fine splittings) are predicted to be smaller than the experimental data in perturbative predictions of the heavy quarkonium energy levels. This tendency is reflected in our analysis in the differences of the determined values of $\overline{m}_{b,c}$ from the different spin states. There have been studies that particular higher-order corrections increase the splittings (hence, tend to remedy the differences), namely the corrections originating from the running of α_s [32] and from resummation of ultra-soft logarithms by the RG equation of potential-NRQCD EFT [33]. We did not include these corrections specific to the heavy quarkonium energy levels in our estimates of higher-order corrections. Rather we used more general methods applied in estimates of unknown higher-order corrections for various physical observables. We remark that, in the end, we obtain consistent error estimates in both ways.

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[§] Calculation procedures were less systematized and unclear, when the same method was applied more than a decade ago up to NNLO.

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